

Generative Retrieval as Multi-Vector Dense Retrieval

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ABSTRACT

For a given query generative retrieval generates identifiers of relevant documents in an end-to-end manner using a sequence-to-sequence architecture. The relation between generative retrieval and other retrieval methods, especially those based on matching within dense retrieval models, is not yet fully comprehended. Prior work has demonstrated that generative retrieval with atomic identifiers is equivalent to single-vector dense retrieval. Accordingly, generative retrieval exhibits behavior analogous to hierarchical search within a tree index in dense retrieval when using hierarchical semantic identifiers. However, prior work focuses solely on the retrieval stage without considering the deep interactions within the decoder of generative retrieval.

In this paper, we fill this gap by demonstrating that generative retrieval and multi-vector dense retrieval share the same framework for measuring the relevance to a query of a document. Specifically, we examine the attention layer and prediction head of generative retrieval, revealing that generative retrieval can be understood as a special case of multi-vector dense retrieval. Both methods compute relevance as a sum of products of query and document vectors and an alignment matrix. We then explore how generative retrieval applies this framework, employing distinct strategies for computing document token vectors and the alignment matrix. We have conducted experiments to verify our conclusions and show that both paradigms exhibit commonalities of term matching in their alignment matrix.

Our findings apply to many generative retrieval identifier designs and provide possible explanations on how generative retrieval can

express query-document relevance. As multi-vector dense retrieval is the state-of-the-art dense retrieval method currently, understanding the connection between generative retrieval and multi-vector dense retrieval is crucial for shedding light on the underlying mechanisms of generative retrieval and for developing, and understanding the potential of, new retrieval models.

CCS CONCEPTS

• Information systems → Retrieval models and ranking.

KEYWORDS

Generative Retrieval; Dense Retrieval; Multi-Vector Dense Retrieval

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1 INTRODUCTION

In recent years, the advent of pre-trained language models has catalyzed the popularity of neural-based retrieval models within the information retrieval community [13, 14, 29, 32, 38].

Neural-based retrieval models. One family of effective neural-based retrieval methods, *dense retrieval* (DR), has achieved the state-of-the-art ranking performance on multiple benchmarks [13, 14, 29]. Several approaches have been proposed to use multiple vectors to represent documents or queries, a.k.a., *multi-vector dense retrieval* (MVDR) [14, 32, 48].

Recently, *generative retrieval* (GR) has emerged as a new paradigm in information retrieval. It aims to generate identifiers of relevant documents for a given query directly and parametrizes the indexing, retrieval, and ranking process in dense retrieval systems

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into a single model. GR adopts a sequence-to-sequence architecture model and is trained to directly map queries to their relevant document identifiers.

Generative retrieval vs. dense retrieval. Dense retrieval models typically employ encoders, e.g., BERT [6], for encoding both queries and documents, while the generative retrieval model adopts an encoder for query encoding and a decoder for identifier generation. Despite their superficial differences, dense retrieval and generative retrieval share key characteristics in their query-document relevance computations. When the two methods use document identifiers such as sub-strings, titles, or semantic IDs as representations for documents, both methods compute relevance to a query of a document as the dot product of two vectors. Dense retrieval involves using the direct product of the query vectors and document vectors as the relevance, while generative retrieval leverages the product of the last latent state from the decoder at each position with the prediction head, a.k.a., the word embedding lookup table. Consequently, a natural question that arises in this context:

How is generative retrieval related to dense retrieval?

Although GR has shown promising results in various benchmarks as a new end-to-end retrieval paradigm [18, 24, 36, 39, 42], relatively few publications have closely examined how GR models work. Nguyen and Yates [28] have shown that GR using atomic identifiers can be viewed as a variant of bi-encoders for dense retrieval because the word embedding lookup table in generative retrieval works exactly the same as the flat index in dense retrieval. Thus, we can partially respond to the above question that GR with atomic identifiers is single-vector dense retrieval. Although atomic identifiers are considered non-mainstream in GR, it offers an insightful perspective on the matter. Nguyen and Yates [28] also discuss that GR with hierarchical semantic identifiers exhibits behavior similar to hierarchical search within a tree index in dense retrieval. However, their discussion focuses only on the retrieval stage without rigorously considering deep interactions within the decoder.

Generative retrieval as multi-vector dense retrieval. In this work, we connect generative retrieval to a state-of-the-art dense retrieval method, multi-vector dense retrieval, in a rigorous way. We illustrate that these two methods exhibit *commonalities in their training targets and a shared focus on semantic matching*. We first examine the attention layer and the prediction head of GR and show that the logits in the loss function can be reformulated to a product of document word embeddings, query token vectors, and attention matrix in Section 4. This corresponds to the unified MVDR framework introduced in [17, 32]. In Section 5 we explore the distinct document encoding and alignment strategy in GR. Specifically, our discussion includes (i) its simple document encoding and how prefix-aware weight-adaptive (PAWA) decoding [39] and non-parametric (NP)-decoding [16] apply to our framework (Section 5.1), and (ii) the distinct alignment strategy employed by GR compared to MVDR and its properties (Section 5.2).

Our discovery provides reliable explanations of how GR can express query-document relevance. By explaining how the GR method models query-document relevance, we can further understand how GR is fundamentally different from dense retrieval methods and

adds to the spectrum of neural-based retrieval models. The connection we present provides the variants of GR methods with a theoretical foundation for further improvement.

Contributions. Our main contributions in this paper are:

- (1) We offer new insights into GR from the perspective of MVDR by showing that these methods share the same framework for measuring query-document relevance.
- (2) We explore how GR applies this framework, employing distinct strategies for document encoding and the alignment matrix.
- (3) We also conduct extensive analytical experiments based on the framework to verify our conclusions and illustrate the term-matching phenomenon and properties of different alignment directions in both paradigms.

2 RELATED WORK

Multi-vector dense retrieval (MVDR) can be seen as a generalization of single-vector dual encoder models [13, 14]. Instead of encoding the complete content of both query and documents into a single low-dimensional vector, MVDR uses fine-grained token-level modeling for scoring. MVDR models such as ColBERT [14] compute query-document relevance by selecting the highest-scoring document token for each query token and aggregating the scores. The postponed token-level interactions allow us to efficiently apply the model for retrieval, benefiting the effectiveness of modeling fine-grained interactions. MVDR overcomes the limited expressivity of single-vector retrieval and achieves significantly better results across various benchmarks [13, 14, 17, 23, 29, 32]. However, due to the cost of storing vectors for each document token, it is challenging to scale the approach to large collections [9, 14, 17, 32].

Generative retrieval (GR) is an emerging paradigm in information retrieval [18, 31, 34, 38, 39, 45]. It leverages generative models to directly generate identifiers of relevant documents. This approach originated with [2, 38] and has garnered considerable attention [see, e.g., 37]. Currently, all implementations of the generative retrieval paradigm adhere to an encoder-decoder transformer architecture, e.g., T5 [33] and BART [19]. In this method, documents are initially associated with a concise token sequence that serves as an identifier. The model is then trained to predict this token sequence autoregressively, using conventional cross-entropy loss.

One notable advantage of the generative retrieval model is its streamlined end-to-end architecture, which requires significantly less disk storage space compared to other retrieval methods. However, it is important to note that due to the limited supervision of each token, the generative retrieval may not achieve comparable performance when compared to dense retrieval [31, 44].

Connecting dense retrieval and generative retrieval. Nguyen and Yates [28] show that GR with atomic identifiers is equivalent to single-vector dense retrieval. They compare the inferential processes of DR with a tree index and GR with hierarchical identifiers. However, the former is just an optimized version of the original DR without changing the semantic matching method, while the latter also considers the predicted IDs and the query in each generation step, which greatly affects how GR would express the relevance, but this is ignored in [28]. Yuan et al. [44] empirically analyze the error rate at each generation step of GR and identify the problem

of poor memory accuracy for fine-grained features compared with DR. They integrate GR and DR into a new coarse-to-fine retrieval paradigm, combining their respective strengths, but circumvented an in-depth discussion of the connection.

In this work, we address the limitations listed above by showing that GR expresses query-document relevance in the same way as MVDR. This connection is rigorously derived from the decoder of GR and can be applied to many identifiers.

3 PRELIMINARIES

In this section, we formulate our task and introduce key notation and the mainstream framework of MVDR models.

Task definition. We formulate the retrieval task as ranking by relevance score. Given a query q , we aim to retrieve relevant documents d in \mathcal{D} by ranking them by their relevance $\text{rel}(d, q)$ to q .

Notation. Table 1 lists the main notation used in the paper. We denote the word embedding lookup table in the decoder as \mathbf{E} and the vocabulary set as \mathcal{V} . Each document d comprises M tokens. To ensure uniform length, padding tokens are added or excess tokens are truncated from each document. The word embedding matrix of d is denoted as $\mathbf{E}_d := [e_{d_1}, \dots, e_{d_M}] \in \mathbb{R}^{d \times M}$, and the latent token vector matrix after encoding is $\mathbf{D} := [d_1, \dots, d_M] \in \mathbb{R}^{d \times M}$. Each query q with N tokens has token vectors $\mathbf{Q} := [q_1, \dots, q_N] \in \mathbb{R}^{d \times N}$ after encoding, similar to the documents.

Table 1: Main notation used in this work.

Symbol	Description
\mathbf{E}	word embedding lookup table
\mathbf{E}_d	document word embedding matrix
\mathbf{D}, \mathbf{Q}	document / query token vector matrix
d_i, q_j	document / query tokens
\hat{d}_i, \hat{q}_j	encoded document / query token vector

Framework for MVDR. Following [17, 32], MVDR methods can be represented as a unified framework, in which the relevance to query q of document d is given by:

$$\text{rel}(d, q) = \frac{1}{Z} \text{sum}(\mathbf{D}^\top \mathbf{Q} \odot \mathbf{A}) = \frac{1}{Z} \sum_{i,j} \hat{d}_i^\top \hat{q}_j A_{ij}, \quad (1)$$

where \mathbf{A} is the alignment matrix that controls whether a document and query token pair can be matched and contribute to the relevance, and $Z = \sum_{i,j} A_{ij}$ is used for normalization and is dropped in many MVDR methods.

Alignment strategy. Different MVDR models adopt different alignment strategies, and, thus, a different alignment matrix \mathbf{A} . It is often computed using heuristic algorithms, such as lexical exact match [11], top-1 relevant token match [14], single-vector alignment [13, 25], or sparse unary salience [32].

Contrastive loss used in MVDR. MVDR methods usually use contrastive loss as the training target, where negative documents are used. For a query q and target document d , the loss is computed as

$$\mathcal{L}(d, q) = -\log \frac{\exp \text{rel}(d, q)}{\sum_{d^- \in \mathcal{D}^-} \exp \text{rel}(d^-, q)}, \quad (2)$$

where \mathcal{D}^- is the collected negative set.

4 IN-DEPTH ANALYSIS OF GENERATIVE RETRIEVAL

To address the question posed in Section 1, this section conducts a detailed analysis of GR. Specifically, we first illustrate the model architecture and training loss of the GR (Section 4.1). Subsequently, we derive that the training target of GR falls into the framework of MVDR (Section 4.2):

$$\mathcal{L}(d, q) \propto \text{sum} \left(\tilde{\mathbf{E}}_d^\top \mathbf{Q} \odot \mathbf{A} \right), \quad (3)$$

where $\tilde{\mathbf{E}}_d$, \mathbf{Q} and \mathbf{A} correspond to \mathbf{D} , \mathbf{Q} and \mathbf{A} in Eq. (1).

4.1 Model architecture and training loss

Model architecture. We focus on the transformer sequence-to-sequence architecture used in GR, more precisely, the encoder-decoder structure. Within this framework, the encoder primarily targets processing the input query, while the decoder is tasked with predicting document identifiers.

The decoder component consists of stacks of self-attention, cross-attention, and feed-forward layers. We particularly underscore the significance of the cross-attention layers, as they facilitate interaction between query tokens and document tokens.

To predict the document token d_i at the i -th position, we compute the cross attention weights between query token vectors \mathbf{Q} and \hat{d}_{i-1} from the previous attention layers at position $(i-1)$ as follows:

$$\alpha_i = \text{softmax}(\mathbf{Q}^\top \mathbf{W} \hat{d}_{i-1}), \quad (4)$$

where $\text{softmax}(\cdot)$ denotes the column-wise softmax function, $\mathbf{W} \in \mathbb{R}^{d \times d}$ is the product of the attention matrices \mathbf{W}_K and \mathbf{W}_Q , i.e., $\mathbf{W} = \mathbf{W}_K^\top \mathbf{W}_Q$, and $\alpha_i \in \mathbb{R}^N$.

Consequently, the output of the cross-attention layer is

$$\mathbf{h}_i = \mathbf{W}_V \mathbf{Q} \alpha_i \in \mathbb{R}^d. \quad (5)$$

For simplicity, we ignore the non-linear activation functions, and the linear maps in the feedforward layers can be absorbed in attention weights, e.g., \mathbf{W}_V . Therefore, \mathbf{h}_i serves as the prediction head for generating the next token.

Training loss. The loss function to minimize at position i is formulated as:

$$\mathcal{L}_i(d, q) = -\log \left(\frac{\exp e_{d_i}^\top \mathbf{h}_i}{\sum_{v \in \mathcal{V}} \exp e_v^\top \mathbf{h}_i} \right) \quad (6)$$

$$= -e_{d_i}^\top \mathbf{h}_i + \log \sum_{v \in \mathcal{V}} \exp e_v^\top \mathbf{h}_i. \quad (7)$$

4.2 GR has the same framework as MVDR

Next, we demonstrate that GR shares a similar framework with MVDR, namely, that the logits within the loss function can be reformulated as a product of document word embeddings, query token vectors, and attention matrix. This formulation corresponds to Eq. (1).

In particular, as we employ teacher-forcing supervision, ground-truth document identifiers are directly fed into the decoder, and token vectors at all positions are computed simultaneously. Based

on this configuration, the overall loss is given by:

$$\mathcal{L}(d, q) = \sum_{i \in [M]} \log p(d_i | d_{i-1}, \dots, d_0, q) \quad (8)$$

$$= \sum_{i \in [M]} \mathcal{L}_i(d, q) \quad (9)$$

$$= \sum_{i \in [M]} \left(-e_{d_i}^\top \mathbf{h}_i + \log \sum_{v \in \mathcal{V}} \exp e_v^\top \mathbf{h}_i \right), \quad (10)$$

where d_0 could be some special token such as [BOS] or the [CLS] token vector from the query.

When using the sampled softmax loss, which involves employing several negative tokens instead of the entire set of tokens in the lookup embedding table, the loss exhibits a similar structure to the contrastive loss used in DR and MVDR. Consequently, we treat the dot product of embedding e_{d_i} and token vector \mathbf{h}_i , i.e., $e_{d_i}^\top \mathbf{h}_i$, as the final relevance score at position i . Further insights into the reason are elaborated in Appendix A. We plug in the dot product with the computation of \mathbf{h}_i from Eq. (5) and obtain:

$$\text{rel}(d, q) = \sum_{i \in [M]} e_{d_i}^\top \mathbf{h}_i \quad (11)$$

$$= \sum_{i \in [M]} e_{d_i}^\top \mathbf{W}_V \mathbf{Q} \alpha_i \quad (12)$$

$$= \sum_{i \in [M]} \sum_{j \in [N]} \tilde{e}_{d_i}^\top \mathbf{q}_j \alpha_{ij} \quad (13)$$

$$= \text{sum} \left(\tilde{\mathbf{E}}_d^\top \mathbf{Q} \odot \mathbf{A} \right), \quad (14)$$

where $\tilde{e}_{d_i}^\top = e_{d_i}^\top \mathbf{W}_V$, $\tilde{\mathbf{E}}_d^\top = \mathbf{E}_d^\top \mathbf{W}_V$, $\mathbf{A} = [\alpha_1, \dots, \alpha_M]^\top \in \mathbb{R}^{M \times N}$, and \odot is the element-wise matrix product operation.

Further, we have a more detailed computation

$$\text{rel}(d, q) = \text{sum} \left(\tilde{\mathbf{E}}_d^\top \mathbf{Q} \odot \mathbf{A} \right) \quad (15)$$

$$= \text{sum} \left(\tilde{\mathbf{E}}_d^\top \mathbf{Q} \odot \text{softmax} \left(\hat{\mathbf{D}}_{-1}^\top \mathbf{W}^\top \mathbf{Q} \right) \right), \quad (16)$$

where $\hat{\mathbf{D}}_{-1} = [\hat{d}_0, \hat{d}_1, \dots, \hat{d}_{M-1}]$ is the output from the previous layer with the right-shifted document tokens as model input.

In conclusion, for GR we observe a similar framework as for MVDR, $\text{rel}(d, q) = \text{sum}(\tilde{\mathbf{E}}_d^\top \mathbf{Q} \odot \mathbf{A})$, where relevance is represented by an interaction of multiple “token vectors,” i.e., $\tilde{\mathbf{E}}_d$ and \mathbf{Q} , from both query and document and aligned by a matrix \mathbf{A} . We summarize our derivation and conclusion in Figure 1.

5 COMPARISON BETWEEN MVDR AND GR

To further explore how GR is related to MVDR, we build upon the unified framework of relevance computation for GR and MVDR derived in the previous section. We conduct a comprehensive analysis of both methods, focusing specifically on their similarities and disparities in terms of the document encoding and the design of the alignment matrix. A summary of the comparison between the two methods is shown in Table 2.

MVDR relevance computation

$$\text{rel}(d, q) = \sum \text{top-k}(D^\top Q) = \sum_{ij} \left(\begin{array}{c} D^\top Q \\ \odot \\ \begin{array}{c} \text{column-wise} \\ \text{top-k} \\ \mathbf{A} (\text{Sparse}) \end{array} \end{array} \right)$$

GR training loss

$$\mathcal{L}(d, q) \propto \sum e_{d_i}^\top \mathbf{h}_i = \sum_i \left(\begin{array}{c} e_{d_i}^\top \\ \times \\ \mathbf{q}_1 \mathbf{q}_2 \dots \mathbf{q}_N \\ \times \\ \alpha_i \end{array} \right)$$

$$= \sum_{ij} \left(\begin{array}{c} \mathbf{E}_d^\top Q \\ \odot \\ \mathbf{A} (\text{Dense}) \end{array} \right)$$

Legend:

- : doc embed vec
- : query token vec
- : cross attention

Figure 1: Summary of our derivation and conclusion. The logits of GR can be reformulated as $\text{sum}(\mathbf{E}_d^\top \mathbf{Q} \odot \mathbf{A})$, which corresponds to the framework $\text{sum}(D^\top Q \odot A)$ of MVDR.

Table 2: Summary of our comparison between MVDR and GR.

Component in	Model		Comparison
$\text{sum}(D^\top Q \odot A)$	MVDR (Sect. 3)	GR (Sect. 4)	
D doc token	D (token vec.)	\tilde{E}_d (embed. vec.)	Sect. 5.1
Q query token	Q (token vec.)	Q (token vec.)	–
A alignment matrix	sparse query-to-doc	dense and learned doc-to-query	Sect. 5.2

5.1 Document encoding

One of the noticeable differences between GR and MVDR is in the document encoding. As depicted in Figure 1, MVDR uses more expressive contextualized token vectors $D = [d_1, \dots, d_M]$ for each position. In contrast, GR only attends each query token to a simple word embedding e_{d_i} that does not hold any contextual information about the document. This was considered a severe compromise for the extremely lightweight modeling and storage of GR. To address this imbalance in modeling capacity, several studies [16, 39] have proposed novel decoding methods. Wang et al. [39] introduce the prefix-aware weight-adaptive (PAWA) decoding method, while Lee et al. [16] propose the non-parametric (NP) decoding. We incorporate these methods into our framework and show how they fundamentally improve the encoding compared with MVDR in Table 3.

Table 3: Document encoding comparison between GR and MVDR. PAWA and NP-decoding either multiply or replace the simple embedding vectors \tilde{E}_d with contextualized token vectors \hat{D} .

Model	Document encoding
MVDR (Sect. 3)	D (token vec.)
GR (Sect. 4)	\tilde{E}_d (embed. vec.)
– w/ PAWA	$\tilde{E}_d \rightarrow \tilde{E}_d \hat{D}'$ (embed. & token vec.)
– w/ NP-dec.	$\tilde{E}_d \rightarrow D$ (token vec.)

PAWA enhances the document encoding from $\tilde{\mathbf{E}}_d$ to $\tilde{\mathbf{E}}_d \tilde{\mathbf{D}}'$. PAWA [39] aims to improve the embedding modeling for distinguishing different semantics of a token ID at different positions. Unlike the standard transformer, which uses a static embedding lookup table for every position, PAWA generates different embedding tables at each generation step. PAWA consists of a transformer decoder and an adaptive projection layer $\mathbf{E} \in \mathbb{R}^{M \times |\mathcal{V}| \times d \times d}$. The projection matrix of token v at the i -th position is

$$\mathbf{E}_{i,v} = \mathbf{E}[i, v, :, :] \in \mathbb{R}^{d \times d}.$$

Here, \mathbf{E} can be seen as a generalized version of the embedding lookup table that uses a matrix $\mathbf{E}_{i,v}$ to represent each token v . To get the generated embedding vector for token v at the i -th position, PAWA decoder first uses the transformer decoder to process the document into a set of latent vectors $\mathbf{D}' = [d'_1, \dots, d'_M] \in \mathbb{R}^{d \times M}$. Then it multiplies the projection matrix $\mathbf{E}_{i,v}$ with the latent vector d'_i and gets the final embedding vector $e_{i,v} = \mathbf{E}_{i,v} d'_i$.

Therefore, we have the logit $e_v^\top \mathbf{h}_i$ in loss Eq. (10) replaced by $e_{i,v}^\top \mathbf{h}_i = d_i'^\top \mathbf{E}_{i,v}^\top \mathbf{h}_i$:

$$\mathcal{L}(d, q) = \sum_{i \in [M]} \left[-d_i'^\top \mathbf{E}_{i,d_i}^\top \mathbf{h}_i + \log \sum_{v \in \mathcal{V}} \exp d_i'^\top \mathbf{E}_{i,v}^\top \mathbf{h}_i \right]. \quad (17)$$

With a similar derivation as in Section 4.2, the relevance can be established as

$$\text{rel}(d, q) = \text{sum} \left(\tilde{\mathbf{D}}'^\top \tilde{\mathbf{E}}_d^\top \mathbf{Q} \odot \mathbf{A} \right), \quad (18)$$

where

$$\tilde{\mathbf{D}}' = \begin{bmatrix} d'_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & d'_2 & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & d'_M \end{bmatrix} \in \mathbb{R}^{(d \times M) \times M}, \quad (19)$$

and $\tilde{\mathbf{E}}_d = \mathbf{W}_V^\top [\mathbf{E}_{1,d_1}, \dots, \mathbf{E}_{M,d_M}] \in \mathbb{R}^{d \times (d \times M)}$.

As we can see, PAWA multiplies the term $\tilde{\mathbf{E}}_d^\top \mathbf{Q}$ with contextualized document token vectors $\tilde{\mathbf{D}}'$, which greatly improves the expressivity of document encoding.

NP-decoding directly replaces $\tilde{\mathbf{E}}_d$ with \mathbf{D} . Lee et al. [16] employ an approach akin to contextualized sparse retrieval methods, leveraging token vectors encoded by the Contextualized Embedding Encoder [CE Encoder, 16], referred to as contextualized token embeddings. This set of vectors, written as \mathbf{D} in our notation, serves as the embedding table for the decoder. Both the BASE and ASYNC non-parametric decoding methods in [16] can be reformulated within our framework as:

$$\text{rel}(d, q) = \text{sum}(\mathbf{D}^\top \mathbf{Q} \odot \mathbf{A}), \quad (20)$$

where \mathbf{D} are the token vectors of documents either pre-computed (as done by the pre-trained T5 model and frozen in the BASE method) or gradually updated (by the encoder of the GR model every N epochs in the ASYNC method) during the training of the GR model.

While the NP-decoding method shares the same document encoding with MVDR, two significant differences exist:

- (1) In NP-decoding, \mathbf{D} is mostly frozen and detached from training, causing training imbalance compared to MVDR. \mathbf{Q} and \mathbf{A} in NP-decoding are fully trained, while \mathbf{D} remains frozen.
- (2) Due to GR computing logits for the entire vocabulary in each generation step, there is a need to reduce the large storage footprint of \mathbf{D} to save computation. NP-decoding methods address this by using clustering to compress token vectors. MVDR, on the other hand, achieves lower inference time through a sparse alignment strategy.

5.2 Alignment strategy

In addition to document encoding, the alignment matrix represents a crucial distinction between GR and MVDR methods. This matrix plays a decisive role in shaping the divergent inference procedures employed in retrieval. In this section, we analyze the alignment matrix, denoted as \mathbf{A} within our unified framework, in terms of sparsity, alignment direction, and some common properties.

5.2.1 The concept of “alignment” in both methods. The concept of “alignment” has garnered significant attention in MVDR [8, 17, 22, 32]. We will briefly introduce the alignment problem in MVDR models, and claim that the alignment matrix of the GR method, as asserted in our framework Eq. (16), indeed exhibits similar alignment functionality to MVDR models.

Token alignment involves determining whether tokens from the query and document should be matched lexically or semantically. It essentially represents another formulation of the “term mismatch problem” [9, 14, 32, 47]. The prevailing strategy considered optimal at present is the all-to-all soft alignment strategy in MVDR models [14, 32], which eliminates the lexical form match restriction.

GR methods leverage the transformer architecture that originated in NLP, and the concept of “alignment” has been extensively discussed in the domain of neural machine translation [3, 5, 20, 21], focusing on the alignment between tokens in source and target sentences. The attention mechanism, as a core component, computes the alignment matrix and proves highly effective in capturing alignment between source and target sentences [5, 12, 43, 46]. Theoretical work [7, 30] has validated the phenomenon of copying behavior, forming a foundational basis for the alignment ability.

We conclude that, in GR methods, the attention matrix is able to capture the alignment between the query and the document, akin to the alignment matrix observed in MVDR methods.

5.2.2 Different sparsity and learnability: sparse vs. dense and learned alignment matrices. The alignment matrices of MVDR and GR differ in sparsity and learnability. MVDR typically employs a sparse alignment matrix for maximum efficiency during inference. In contrast, GR uses a dense and fully learnable alignment matrix derived from the computationally intensive attention mechanism.

For MVDR methods, the sparse alignment matrix is often computed using heuristic algorithms [11, 14, 32]. Taking ColBERT [14] as an example, it selects the most relevant document token for each query token. The relevance score between document d and query

q is computed as

$$\begin{aligned} \text{rel}(d, q) &= \text{sum}(\mathbf{D}^\top \mathbf{Q} \odot \mathbf{A}) = \sum_{i,j} \mathbf{d}_i^\top \mathbf{q} A_{ij} \\ &= \sum_{j \in [N]} \max_{i \in [M]} \mathbf{d}_i^\top \mathbf{q}_j = \sum_{j \in [N]} \text{rel}(d, q_j), \end{aligned} \quad (21)$$

where \mathbf{A} is a sparse alignment matrix with only one non-zero element for each column ($A_{ij} = 1$ if $\mathbf{d}_i^\top \mathbf{q}_j = \max_{i \in [M]} \mathbf{d}_i^\top \mathbf{q}_j$; $A_{ij} = 0$ otherwise). The sum-max operation is highly parallelizable, ensuring efficiency during inference.

For GR methods, the alignment matrix is computed through the attention mechanism, considering all possible pairs of query and document tokens, as shown in Eq. (16).

The dense alignment matrix is highly expressive and trainable. While not suitable for exact relevance score computation in inference for each query-document pair, efficient approximate algorithms such as greedy search or beam search can be used to retrieve the top- k documents. These decoding algorithms rely on the following decomposition:

$$\text{rel}(d, q) = \sum_{i \in [M]} \text{sum}(\hat{\mathbf{e}}_{d_i}^\top \mathbf{Q} \alpha_i) = \sum_{i \in [M]} \text{rel}(d_i, q), \quad (22)$$

where $\text{rel}(d_i, q)$ is conditioned on d_0, \dots, d_{i-1} , approximating the search for the most relevant document d to finding the most relevant token d_i at each position i .

5.2.3 Different alignment directions: query-to-document vs. document-to-query alignment. Beyond differences in the sparsity and learnability of the alignment matrix, MVDR and GR exhibit distinctions in their alignment directions.

Eq. (21) reveals that MVDR's relevance score can be decomposed into the sum of relevance scores for each query token and its aligned document token. In this context, we consider the alignment matrix in MVDR as **query-to-document** alignment. Each query token individually aligns to a document token, seeking the optimal match during retrieval. Mathematically, the alignment matrix is computed *column-wise* and represents a one-hot vector for each column.

Conversely, the relevance score of GR, as depicted in Eq. (22), is the sum of relevance scores for each document token and its softly aligned query token. Here, we categorize the alignment matrix in GR as **document-to-query** alignment. Each document token is considered individually to focus attention on the most relevant query token. The alignment matrix is computed *row-wise* with a $\text{softmax}(\cdot)$ operation to normalize attention weights in each row.

Document-to-query alignment may seem counter-intuitive for a retrieval task, as we do not know the target documents while predicting. As a solution, GR pre-computes the alignment strategy for the document token d_i (to be predicted) using *previous* document tokens d_0, \dots, d_{i-1} and thus can retrieve the next token that best aligns with the desired *next* alignment strategy.

5.2.4 Low-rank nature of both alignment matrices. In analyzing the shared characteristics of the two alignment matrices, it is demonstrated that both matrices exhibit a low-rank property.

MVDR models, e.g., ALIGNER [32], integrate the pairwise alignment matrix with unary salience, given by

$$\mathbf{A} = \tilde{\mathbf{A}} \odot \mathbf{u}_d \mathbf{u}_q^\top. \quad (23)$$

Here, $\tilde{\mathbf{A}} \in \mathbb{R}^{M \times N}$ signifies the pairwise alignment matrix, determining the alignment of query and document tokens. The sparse token weights, $\mathbf{u}_d \in \mathbb{R}^M$ and $\mathbf{u}_q \in \mathbb{R}^N$, decide whether a token requires alignment. Notably, the alignment matrix \mathbf{A} contains a low-rank component $\mathbf{u}_d \mathbf{u}_q^\top$ that influences the alignment strategy.

In the case of GR methods, the alignment matrix is computed using an attention mechanism, which inherently results in a low-rank matrix. A lemma provides evidence of this low-rank property and is presented briefly here, with a detailed proof delegated to Wu et al. [41, Appendix B] due to space limitations.

LEMMA 5.1. *For a matrix $\mathbf{A} = \text{softmax}(\mathbf{D}^\top \mathbf{W} \mathbf{Q})$, there exists a rank-one matrix \mathbf{R} such that*

$$\|\mathbf{A} - \mathbf{R}\| \leq 4\gamma \|\mathbf{W}\|, \quad (24)$$

where the term γ depends on the matrix entries.

From this lemma, we can conclude that both MVDR and GR methods reveal a rank-one component in their alignment matrices.

5.2.5 Decomposition of both relevance scores. In this subsection, we show that the relevance score computation in both MVDR and GR models can be decomposed into query and document components.

The MVDR method employs a bi-encoder architecture, wherein query and document tokens are modeled separately. This architecture can easily be regarded as a decomposition of the relevance score between the query and document:

$$\text{rel}(d, q) = \text{sum}(\mathbf{D}^\top \mathbf{Q} \odot \mathbf{A}) = \text{sum}(\text{top-1}(\mathbf{D}^\top \mathbf{Q})),$$

where $\text{top-1}(\cdot)$ is the operator that selects the maximum value in each column of the matrix.

In the subsequent lemma, we establish that the relevance score of GR cannot only be decomposed but also be kernelized, implying the existence of a kernel function capable of processing both query vectors and document vectors to compute the score (further details are delegated to Wu et al. [41, Appendix C] due to space limitations):

LEMMA 5.2. *For simplicity, let $\text{rel}(d, q) = \text{sum}(\mathbf{D}^\top \mathbf{Q} \odot \mathbf{A})$, where $\mathbf{A} = \text{softmax}(\mathbf{D}^\top \mathbf{Q})$. It can be kernelized as*

$$\begin{aligned} \text{rel}(d, q) &= \sum_{i,j} \mathbf{d}_i^\top \mathbf{q}_j A_{ij} = \sum_{i,j} \mathbf{d}_i^\top \mathbf{q}_j \text{softmax}(\mathbf{d}_i^\top \mathbf{Q})_j \\ &= \sum_{i,j} \frac{1}{p_{ij}} \text{tr}(\mathbf{F}(\mathbf{d}_i)^\top \mathbf{F}(\mathbf{q}_j)), \end{aligned} \quad (25)$$

where $\mathbf{F}(\mathbf{x}) = \mathbf{x} \phi(\mathbf{x})^\top$, and p_{ij} is a term that depends on \mathbf{d}_i and \mathbf{q}_j . We choose $\text{elu}(\cdot)$ as the kernel function $\phi(\cdot)$.

Furthermore, by applying the trace inequality, we can approximately decompose the relevance score as

$$\text{rel}(d, q) \leq \sum_{i,j} \frac{1}{\hat{p}_i \hat{p}_j} \sqrt{\text{tr}(\mathbf{F}(\mathbf{d}_i)^\top \mathbf{F}(\mathbf{d}_i))} \sqrt{\text{tr}(\mathbf{F}(\mathbf{q}_j)^\top \mathbf{F}(\mathbf{q}_j))}.$$

From this lemma, we can conclude that both relevance scores in MVDR and GR methods can be decomposed. The decomposition of MVDR is more straightforward, and the kernelization of GR is more complicated. Both kernelizations would provide possibilities for new retrieval strategies.

5.3 Upshot

In summary, our findings indicate that certain studies enhance the modeling capacity of GR by employing more expressive document encoding, akin to MVDR. Furthermore, GR employs a distinct alignment direction, but it also exhibits similar low-rank and decomposition properties as MVDR.

6 EXPERIMENTAL SETUP

Next, we seek experimental confirmation that generative retrieval and multi-vector dense retrieval share the same framework for measuring relevance to a query of a document, as derived in Section 4.

6.1 Datasets

We conduct experiments on two well-known datasets, NQ [15] and MS MARCO [27]. We use the same settings and processed datasets as Sun et al. [36], and we summarize the statistics of the datasets in Table 4.

Table 4: Statistics of datasets used in our experiments.

Dataset	# Docs	# Test queries	# Train pairs
NQ320K	109,739	7,830	307,373
MS MARCO	323,569	5,187	366,235

NQ320k. NQ320K is a popular dataset for evaluating retrieval models [13, 24, 38, 39]. It is based on the Natural Questions (NQ) dataset [15]. NQ320k consists of 320k query-document pairs, where the documents are gathered from Wikipedia pages, and the queries are natural language questions.

MS MARCO. The MS MARCO document retrieval dataset is a collection of queries and web pages from Bing searches. Like NQ320k and following [36], we sample a subset of documents from the labeled documents and use their corresponding queries for training. We evaluate the models on the queries of the MS MARCO dev set and retrieval on the sampled document subset.

6.2 Base models

As we aim to provide a new perspective on GR as MVDR, we consider representative models from both paradigms, i.e., SEAL [1] for GR and ColBERT [14] for MVDR. For a fair comparison, we reproduce both methods using the T5 architecture [33]. We have made several changes to adapt ColBERT and SEAL to their T5 variants:¹

- **T5-ColBERT.** We use in-batch negative samples instead of the pair-wise samples in the official ColBERTv1 implementation. We set the batch size to 256 and train 5 epochs. Due to space limitations, details of our T5 variant ColBERT are delegated to Wu et al. [41, Appendix D].
- **T5-SEAL.** We use the Huggingface transformers library [40] to train the model. We use the constructed query-to-span data for training and each span has a length of 10 sampled according to Bevilacqua et al. [1]. The learning rate is set to 1e-3 and the batch size is 256.

¹Our code link is <https://github.com/Furyton/GR-as-MVDR>.

6.3 Inference settings

We consider two inference settings: end-to-end and re-ranking.

End-to-end retrieval setting. Both methods can perform an end-to-end retrieval on the corpus for a given query.

- **T5-ColBERT** maintains a large vector pool of all document token vectors after training. During inference, it first retrieves for each query token vector, the k -nearest document token vectors in the vector pool, resulting in $N \times k$ retrieved vectors. These vectors are from at most $N \times k$ different documents which are used as candidates. It then computes the exact relevance score for each candidate document and performs the final re-ranking.
- **T5-SEAL** directly uses its generative style inference with the help of constrained beam search to predict valid document identifiers, i.e., n-grams from the documents.

Re-ranking setting. Since we are focusing on relevance computing in the training target, we introduce a re-ranking setting that removes the influence of different approximated inference strategies. As stated in some previous work [17, 24], both MVDR and GR have discrepancies between training and inference. The approximated retrieval methods are largely different from the training target and may decrease the performance of the trained retrievers. In the re-ranking setting, we collect 100 documents retrieved by BM25 [35] together with the ground-truth document as the candidate set for each query. As in the training stage, we take both the query and each candidate document as the input of the model and use the relevance computing in Section 3 and 4.

7 EXPERIMENTAL ANALYSES

7.1 Performance of different alignment directions

As described in Section 5.2.3, MVDR and GR exhibit different alignment directions, i.e., query-to-document and document-to-query alignment. We aim to look at how alignment directions affect retrieval performance. We first conduct experiments in the re-ranking setting to show the performance gap between MVDR and GR. As shown in Table 5, MVDR with the original alignment strategy, which is indicated as MVDR (q→d), has a much better performance than GR. To compare the alignment directions of MVDR and GR, we have designed a model MVDR (q←d) that integrates the features of both, i.e., expressive document encoding from MVDR and document-to-query alignment strategy from GR. From Table 5, we can see that the performance of the new model is roughly intermediate between the other two. Note that the designed experimental model MVDR (q←d) can only be used in a re-ranking setting. We conclude that query-to-document alignment is preferred for re-ranking.

7.2 Term matching in alignment

As we have discussed in Section 5.2.1, alignment is essentially a term-matching problem. In this section, we design an experiment to observe the extent of term matching in the two methods, and we find that both methods exhibit a preference for exact term matching in their alignment.

Exact match of MVDR in query-to-document direction. We calculate the exact matching rate between document token IDs and

Table 5: Comparison of MVDR and GR in the re-ranking setting. MVDR and GR are our reproduced T5-SEAL and T5-ColBERT. “R” denotes Recall, and “M” denotes MRR.

Model	NQ320K			MS MARCO		
	R@1	R@10	M@10	R@1	R@10	M@10
MVDR (q→d)	61.3	91.9	72.0	46.5	84.5	58.9
MVDR (q←d)	53.2	90.1	65.7	34.8	78.8	48.4
GR	47.4	87.0	60.5	35.3	77.1	48.3

each query token ID during the alignment process, which we refer to as the “hard exact match rate.” We also define a “soft exact match rate” which is the alignment score corresponding to the exact match query-document token pairs. The alignment score is defined as the element in the alignment matrix. As MVDR uses a sparse alignment matrix, we apply column-wise softmax(\cdot) to \mathbf{A} and use the element as the alignment score. We average the rate over candidate documents for each query token and categorize the query tokens according to their IDF. We assume that IDF approximates the term importance as is done in [10]. From the results in Figure 2, we can see that MVDR chooses exactly matched document tokens in 11.4% on average. Also, we notice that rare query tokens have not received much attention during alignment. This observation suggests that MVDR may prioritize commonly occurring query tokens in its alignment process, potentially overlooking or underemphasizing the importance of rare query tokens.

Exact match of MVDR and GR in document-to-query direction. We have devised an experiment to investigate the alignment in the opposite direction, i.e., document-to-query, in Figure 3. As GR is not trained with hard alignment, we only examine the soft exact match rate of both methods. The computation of the exact match rate is similar except that it is computed for each document token. From the results, we have discerned a consistent trend: as the importance of tokens increases, the rate of exact matches also tends to rise. We think this is because it is hard for the rare query token to match among many common tokens since the document is much longer than the query. When we look at each document token, it will be easier to match among fewer query tokens. We also conduct experiments on MS MARCO and have similar results.

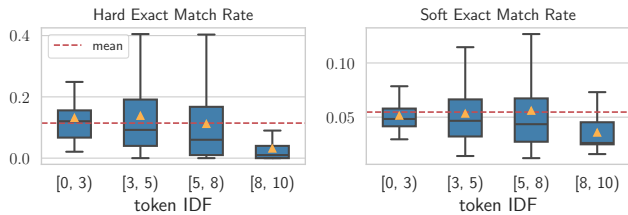


Figure 2: Exact match rate of MVDR on NQ320k dataset in the query-to-document direction.

7.3 Improved document encoding

In Section 5.1, we include two popular document encoding methods, PAWA and NP-decoding, into our framework. To demonstrate the improvement of these two methods, we compare the performance of GR with and without them in Table 6. PAWA is typically used in GR with short semantic identifiers due to its high computational

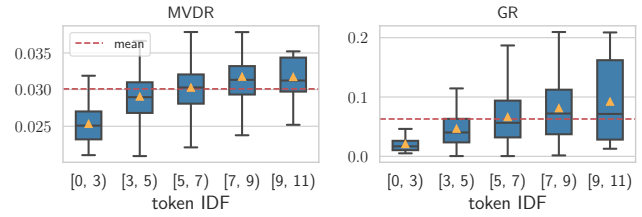


Figure 3: Soft exact match rate of MVDR and GR on NQ320k dataset in the document-to-query direction.

complexity during generation. Thus, we compare it with DSI [38] with semantic identifiers. Note that all these models use the same architecture (T5-base [33]) and similar training procedures without data augmentation, e.g., synthetic query-doc pairs generation, etc. *-PAWA and *-NP can be seen as a naive approach to using the two enhancing methods to the base GR models. From Table 6, we see that both PAWA and NP-decoding can greatly improve the performance and achieve similar results compared with T5-ColBERT on Recall@1. However, there is still a large gap in terms of Recall@10. The implementation of the additional decoding modules is only an approximation for reducing the cost of time and storage as discussed in Section 5.1. This, together with the alignment direction, may be a cause of the performance gap between GR equipped with these document encodings and MVDR.

Table 6: Performance of GR models with different document encoding methods on NQ320k in end-to-end setting. The results of DSI-PAWA, DSI, and T5-GENRE-NP are from [16, 36, 39]. T5-GENRE is the T5 variant of GENRE [2] used by [16].

Model	R@1	R@10
T5-ColBERT	61.1	88.4
DSI [38]	55.2	67.4
DSI-PAWA [39]	60.2	80.2
T5-SEAL	44.7	75.5
T5-GENRE [2]	53.7	64.7
T5-GENRE-NP [16]	62.2	78.8

7.4 Low-rank nature of alignment matrix

In Section 5.2.4, we show that the alignment matrix in GR also has a low-rank property in Lemma 5.1. As MVDR using alignment matrix (23) already contains a low-rank component, we only conduct experiments to verify GR. Since the γ in Lemma 5.1 is hard to attain, we illustrate the relation between $\|\mathbf{W}\|$ and $\|\mathbf{A} - \mathbf{R}\|$ in Figure 4(a). We can see that the inequality is loose and $\|\mathbf{A} - \mathbf{R}\|$ is much lower than $\|\mathbf{W}\|$. We also show the relative error of the approximation of \mathbf{R} in Figure 4(b). The error is relatively low on average, which indicates the low-rank nature of the alignment matrix of GR.

7.5 Case study of the alignment matrix

We chose a specific case from the dataset NQ320k to show what the alignment matrix looks like in Figure 5. Since the document is too long for demonstration, we simplify and extract a sub-sentence containing the answer to the query. In Figure 5(a), we have observed a pronounced phenomenon of exact matches in MVDR. The song name and people’s names are completely matched with high scores.

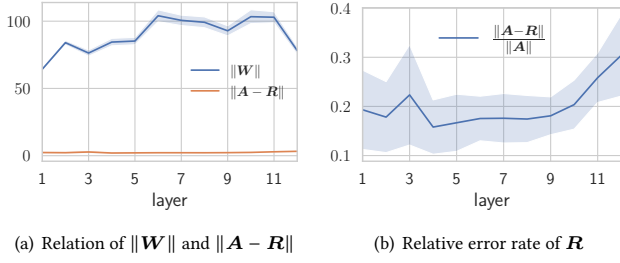


Figure 4: Low-rank approximation of R to alignment matrix A in GR in MS MARCO dataset.



Figure 5: An example of alignment matrix in MVDR and GR.

In Figure 5(b), this phenomenon is less obvious, but each document token has more attention on the people’s name and song name.

7.6 Upshot

We verify the existence of “exact term match,” a specific alignment scenario, in both paradigms. We also show the superiority of the alignment direction in MVDR. The improved document encoding and the low-rank nature of the alignment matrix are validated.

8 LIMITATIONS

We have examined the training target of GR and have connected it with MVDR, but we have not discussed whether relevance computing can be generalized to the generative style inference. We have not considered the multi-layer interactions in the cross-attention between query and document for simplicity.

Our framework does not discuss how query-generation augmentation reduces the discrepancy between training and inference [50]. We aim to study how different architectures and identifier designs will affect the alignment and generalization during inference in future work.

9 CONCLUSION

In this paper, we have offered new insights into GR from the perspective of MVDR that both paradigms share the same frameworks for measuring the relevance between a query and a document. Both paradigms compute relevance as a sum of products of query and document vectors and an alignment matrix. We have explored how GR applies this framework and differs from MVDR. We have shown that GR has simpler document encoding and an alignment strategy with different sparsity and direction. They also share a

low-rank property and can be decomposed into query and document components. We have conducted extensive experiments to verify our conclusions and found that both methods have commonalities of term matching in the alignment. We also found that query-to-document alignment direction has better performance than document-to-query.

Based on our findings, practitioners in the field may consider leveraging the shared frameworks highlighted in this study to understand and develop new GR methods, and pay more attention to the classic term matching problem underlying GR models.

As to future work, we will continue to study how multi-layer attention may affect the framework. The difference in the generalization properties for new documents between DR and GR [4, 26, 28, 49] based on our framework is also an important aspect deserving further investigation. We will continue to discover new relations in the GR paradigm and provide more insights into the methodology.

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A FURTHER EXPLANATION OF THE RELEVANCE SCORE IN GR

Further insights into the reason for using $\sum_{i \in [M]} e_{d_i}^\top \mathbf{h}_i$ as the relevance can be elaborated as follows. Suppose we treat all other token embeddings e_k , where $k \neq d_i$, as fixed with respect to e_{d_i} , then at the early stage of the training, the loss can be expressed as:

$$\mathcal{L}_i(d, q) = -e_{d_i}^\top \mathbf{h}_i + \log \left(\exp e_{d_i}^\top \mathbf{h}_i + \sum_{v \neq d_i} \exp e_v^\top \mathbf{h}_i \right) \quad (26)$$

$$= -e_{d_i}^\top \mathbf{h}_i + \log \left(\exp e_{d_i}^\top \mathbf{h}_i + C \right) \propto -e_{d_i}^\top \mathbf{h}_i. \quad (27)$$

Due to space limitations, details of Appendix A, B, C, and D can be found online in [41].

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